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The Natronomonas pharaonis halorhodopsin (pRH) trimer in a hydrated lipid membrane patch. (A) Monomers A, B, and C depicted as cartoons are colored blue, mauve, and pink, respectively. Chloride ions are shown as green spheres, lipid oxygen atoms are in red, nitrogen in blue, and phosphate atoms are in orange. Lipid tails are depicted as gray bonds. The retinal molecules and K256 side chains are shown as bonds with the carbon atoms in cyan. Hydrogen atoms are not shown. (B) Thickness of the lipid bilayer close to the protein and at remote distances. The thickness of the lipid bilayer is estimated fromthe number density of the lipid phosphorous atoms, computed for lipids within 15 Å of the protein, and for lipids further away from the protein. Each number density is normalized to the number of lipids in the corresponding region. (C) View from the cytoplasmic side of the simulation box. Bacterioruberin is shown as black van der Waals spheres, chloride ions are in green at site-1 and site-2, and retinal with K256 are depicted as yellow van der Waals spheres. Lipid molecules are depicted as van der Waals spheres with carbon atoms in cyan, oxygen — red, nitrogen — blue, and phosphorous atoms in orange. Specific sidechains are depicted using the same color code. (D) Root-mean-squared deviation (RMSD, in Å) of the backbone heavy atoms in the simulation of wild-type halorhodopsin, calculated relative to the starting crystal structure. (E) Close-up view of site-1 in the crystal structure [8] illustrating hydrogen bonding of R123. A.N. Bondar et al., "Electrostatic interactions and hydrogen bond dynamics in chloride pumping by halorhodopsin," Volume 1837/12, pages 1964-1972.

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